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An analytical description of the low temperature behaviour of a weakly interacting Bose gas

Guozhen Su[1,2], **Lixuan Chen**[1,2] **and Jincan Chen**[1,2]

[1] CCAST (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China
[2] Department of Physics, Xiamen University, Xiamen 361005, People's Republic of China

E-mail: gzsu@xmu.edu.cn

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Abstract
An analytical description of the low temperature behaviour of a trapped interacting Bose gas is presented by using a simple approach that is based on the principle of the constancy of chemical potentials in equilibrium and the local-density approximation. Several thermodynamic quantities, which include the ground-state fraction, chemical potential, total energy, entropy and heat capacity, are derived analytically. It is shown that the results obtained here are in excellent agreement with the experimental data and the theoretical predictions based on the numerical calculation. Meanwhile, by selecting a suitable variable, the divergent problem existing in some papers is solved.

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1. Introduction

Bose–Einstein condensation (BEC) is one of the most striking consequences of quantum statistics [1]. The characteristics of BEC may be altered by many factors, which include the number of atoms, the external potential, the dimensionality of space and the interactions between the atoms [2–6], etc. The effects due to the interatomic forces are known to be very small in the normal phase but may become significant when the condensation-induced density increases at low temperatures. A wide variety of BEC properties, such as the size and shape and the energy of the condensate cloud as well as the dispersions of the collective excitation, may be dramatically affected by the interactions [7–11].

The questions of how the interatomic forces affect the low temperature behaviour of Bose systems have become topics of great interest. Early in the 1950s, Huang, Yang and Lee *et al* studied the properties of homogeneous interacting Bose gases based on the two-body pseudopotential [12–15]. Gross, Pitaevskii and Fetter *et al* extended the theory of interacting Bose gases to the inhomogeneous systems [16–19]. Since then many investigations have been done based on the solution of the Gross–Pitaevskii (GP) equation [20–25].

In recent years, a simple approach based on the principle of the constancy of chemical potentials in diffusive equilibrium and the local-density approximation (LDA) has been used to deal with the problem of trapped interacting Bose gases. For example, Oliva [26, 27] used it to explore the density profile of trapped imperfect quantum systems. Similar work was done by Chou *et al* [28]. The approach was also employed by Shi *et al* to derive the thermodynamic properties of a trapped interacting Bose gas [29, 30]. However, the results in [29] are adequate only for $T > T_C$, where T_C is the critical temperature of Bose–Einstein condensation; some equations in [30], as mentioned by the authors, may become useless near the critical temperature because of the divergence.

In the present paper, we will continue to use the simple approach mentioned above to present an analytical description of the low temperature behaviour of a Bose gas trapped in a harmonic potential with repulsive interatomic interactions. Several thermodynamic quantities, which include the ground-state fraction, chemical potential, total energy, entropy and heat capacity, are derived analytically for both the cases of $T \geqslant T_C$ and $T < T_C$. The corrections from the interactions are evaluated up to the first power in a/λ, where a is the s-wave scattering length and $\lambda = \sqrt{2\pi\hbar^2/mk_BT}$ is the thermal wavelength. Meanwhile, by selecting a suitable variable, the divergent problem existing in [30] is solved. It is more important that the analytical results obtained here are in good agreement with the experimental data and the theoretical predictions based on the numerical calculation.

2. Theoretical evaluation

Let us consider a gas of N repulsively interacting bosons trapped in an anisotropic harmonic potential

$$V(\boldsymbol{r}) = \tfrac{1}{2}m\left(\omega_x^2x^2 + \omega_y^2y^2 + \omega_z^2z^2\right) \tag{1}$$

where ω_x, ω_y and ω_z are the angular frequencies of the potential along the x, y, and z directions.

In the presence of an external potential, the spatial distribution of particles is inhomogeneous. Here we extend the theory of interacting Bose gases proposed by Huang, Yang and Lee *et al* [12–15] to the inhomogeneous systems by using the thermodynamic principle that for a system in diffusive equilibrium, the chemical potentials should be constant throughout the system. In turn the chemical potential of the system is given by [26, 27]

$$\mu = \bar{\mu}[n(\boldsymbol{r})] + V(\boldsymbol{r}) \tag{2}$$

where $\bar{\mu}[n(\boldsymbol{r})]$ is the internal chemical potential at $\boldsymbol{r}$, which is generally the non-local functional of density profile $n(\boldsymbol{r})$. If the density varies sufficiently slowly (the condition is often satisfied [28]), we may treat the internal chemical potential within the LDA. Thus, $\bar{\mu}[n(\boldsymbol{r})]$ is taken as a local function of $n(\boldsymbol{r})$, which is of the same form as the chemical potential of a corresponding homogeneous system of density $n(\boldsymbol{r})$. For the weak interactions, i.e., the s-wave scattering length a satisfies $a/\lambda \ll 1$ and $a[n(\boldsymbol{r})]^{1/3} \ll 1$, $\bar{\mu}[n(\boldsymbol{r})]$ derived by Huang, Yang and Lee [15] based on the two-body pseudopotential may be written as

$$\bar{\mu}[n(\boldsymbol{r})] = \begin{cases} k_BT\{\ln \bar{z}_0[n(\boldsymbol{r})] + 4a\lambda^2 n(\boldsymbol{r})\} & [n(\boldsymbol{r}) \leqslant n_C] \\ 2a\lambda^2 k_BT[n_C + n(\boldsymbol{r})] & [n(\boldsymbol{r}) > n_C] \end{cases} \tag{3}$$

where $n_C = \zeta(3/2)/\lambda^3$ is the critical density of particles at which BEC occurs, $\zeta(l) = \sum_{i=1}^{\infty} 1/i^l$ is the Riemann zeta function and $\bar{z}_0[n(\boldsymbol{r})]$ is the non-interacting internal fugacity at $\boldsymbol{r}$, which corresponds to the fugacity of a non-interacting homogeneous Bose system with density $n(\boldsymbol{r})$. $\bar{z}_0[n(\boldsymbol{r})]$ is related to $n(\boldsymbol{r})$ through [15]

$$n(\boldsymbol{r}) = \frac{1}{\lambda^3} g_{3/2}\{\bar{z}_0[n(\boldsymbol{r})]\} \tag{4}$$

where $g_l(x) = \sum_{i=1}^{\infty} x^i / i^l$.

Similarly, under the LDA, the densities of the energy and entropy at r can be, respectively, expressed as

$$u(\boldsymbol{r}) = \bar{u}[n(\boldsymbol{r})] + n(\boldsymbol{r})V(\boldsymbol{r}) \tag{5}$$

and

$$s(\boldsymbol{r}) = \bar{s}[n(\boldsymbol{r})] \tag{6}$$

where $\bar{u}[n(\boldsymbol{r})]$ and $\bar{s}[n(\boldsymbol{r})]$ are the local functions of $n(\boldsymbol{r})$, which are, respectively, given by [15]

$$\bar{u}[n(\boldsymbol{r})] = \begin{cases} k_B T \left\{ \dfrac{3}{2}\dfrac{1}{\lambda^3} g_{5/2}\{\bar{z}_0[n(\boldsymbol{r})]\} + 2a\lambda^2 n^2(\boldsymbol{r}) \right\} & [n(\boldsymbol{r}) \leqslant n_C)] \\ k_B T \left\{ \dfrac{3}{2}\dfrac{1}{\lambda^3}\zeta(5/2) + a\lambda^2\left[2n_C^2 - n(\boldsymbol{r})n_C + n^2(\boldsymbol{r})\right] \right\} & [n(\boldsymbol{r}) > n_C] \end{cases} \tag{7}$$

and

$$\bar{s}[n(\boldsymbol{r})] = \begin{cases} k_B \left\{ \dfrac{5}{2}\dfrac{1}{\lambda^3} g_{5/2}\{\bar{z}_0[n(\boldsymbol{r})]\} - n(\boldsymbol{r}) \ln \bar{z}_0(\boldsymbol{r}) \right\} & [n(\boldsymbol{r}) \leqslant n_C] \\ k_B \left\{ \dfrac{5}{2}\dfrac{1}{\lambda^3}\zeta(5/2) + 3a\lambda^2\left[n_C^2 - n(\boldsymbol{r})n_C\right] \right\} & [n(\boldsymbol{r}) > n_C]. \end{cases} \tag{8}$$

2.1. The case of $T \geqslant T_C$

When $T \geqslant T_C$, all the particles in the system are in the normal states, i.e., $n(\boldsymbol{r}) \leqslant n_C$ throughout the space, so μ, $u(\boldsymbol{r})$ and $s(\boldsymbol{r})$ are, respectively, expressed as

$$\mu = k_B T \{\ln \bar{z}_0[n(\boldsymbol{r})] + 4a\lambda^2 n(\boldsymbol{r})\} + V(\boldsymbol{r}) \tag{9}$$

$$u(\boldsymbol{r}) = k_B T \left\{ \frac{3}{2}\frac{1}{\lambda^3} g_{5/2}\{\bar{z}_0[n(\boldsymbol{r})]\} + 2a\lambda^2 n^2(\boldsymbol{r}) \right\} + n(\boldsymbol{r})V(\boldsymbol{r}) \tag{10}$$

and

$$s(\boldsymbol{r}) = k_B \left\{ \frac{5}{2}\frac{1}{\lambda^3} g_{5/2}\{\bar{z}_0[n(\boldsymbol{r})]\} - n(\boldsymbol{r}) \ln \bar{z}_0(\boldsymbol{r}) \right\} \tag{11}$$

according to equations (2), (3) and (5)–(8). By using the principle of the constancy of chemical potentials, the chemical potential of the system can also be written as

$$\mu = k_B T \{\ln \bar{z}_0[n(0)] + 4a\lambda^2 n(0)\}. \tag{12}$$

If only the terms up to the first power in a/λ are considered, one can derive from equations (4) and (9)–(12) that

$$\mu = k_B T \left[\ln \tilde{z} + \frac{4a}{\lambda} g_{3/2}(\tilde{z}) \right] \tag{13}$$

$$n(\boldsymbol{r}) \approx \frac{1}{\lambda^3} \left\{ g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\} + \frac{a}{\lambda}\{4g_{3/2}(\tilde{z})g_{1/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\} - 4g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}g_{1/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\} \right\} \tag{14}$$

$$u(\boldsymbol{r}) \approx \frac{k_B T}{\lambda^3}\left\{\frac{3}{2}g_{5/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\} + \beta V(\boldsymbol{r})g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\right.$$
$$+\frac{a}{\lambda}\left\{6g_{3/2}(\tilde{z})g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\} - 4g^2_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\right.$$
$$+4\beta V(\boldsymbol{r})g_{3/2}(\tilde{z})g_{1/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}$$
$$\left.\left.-4\beta V(\boldsymbol{r})g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}g_{1/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\right\}\right\} \tag{15}$$

and

$$s(\boldsymbol{r}) \approx \frac{k_B}{\lambda^3}\left\{\frac{5}{2}g_{5/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\} + [\beta V(\boldsymbol{r}) - \ln\tilde{z}]g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\right.$$
$$+\frac{a}{\lambda}\left\{6g_{3/2}(\tilde{z})g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\} - 6g^2_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\right.$$
$$+4[\beta V(\boldsymbol{r}) - \ln\tilde{z}]g_{3/2}(\tilde{z})g_{1/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}$$
$$\left.\left.-4[\beta V(\boldsymbol{r}) - \ln\tilde{z}]g_{3/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}g_{1/2}\{\tilde{z}\exp[-\beta V(\boldsymbol{r})]\}\right\}\right\} \tag{16}$$

where $\beta = 1/k_B T$, $\tilde{z} \equiv \bar{z}_0[n(0)]$ is the non-interacting internal fugacity at the centre of the potential. It is seen from equation (4) that because $n(0) \leqslant n_C$ for $T \geqslant T_C$, $\tilde{z} \equiv \bar{z}_0[n(0)] \leqslant 1$ when $T \geqslant T_C$.

Equations (14)–(16) present, respectively, the spatial distributions of particles, energy and entropy. Substituting the expression of $V(\boldsymbol{r})$ into equations (14)–(16), one can obtain, respectively, the total number of particles, total energy and entropy of the system as

$$N = \int n(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = \left(\frac{k_B T}{\hbar\varpi}\right)^3\left\{g_3(\tilde{z}) + \frac{a}{\lambda}[4g_{3/2}(\tilde{z})g_2(\tilde{z}) - 4F_{3/2,1/2,3/2}(\tilde{z})]\right\} \tag{17}$$

$$U = \int u(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = k_B T\left(\frac{k_B T}{\hbar\varpi}\right)^3\left\{3g_4(\tilde{z}) + \frac{a}{\lambda}[12g_{3/2}(\tilde{z})g_3(\tilde{z}) - 14F_{3/2,1/2,5/2}(\tilde{z})]\right\} \tag{18}$$

and

$$S = \int s(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = k_B\left(\frac{k_B T}{\hbar\varpi}\right)^3\left\{4g_4(\tilde{z}) - \ln\tilde{z}g_3(\tilde{z}) + \frac{a}{\lambda}[12g_{3/2}(\tilde{z})g_3(\tilde{z})\right.$$
$$\left.-4\ln\tilde{z}g_{3/2}(\tilde{z})g_2(\tilde{z}) - 18F_{3/2,1/2,5/2}(\tilde{z}) + 4\ln\tilde{z}F_{3/2,1/2,3/2}(\tilde{z})]\right\} \tag{19}$$

where $\varpi \equiv (\omega_x\omega_y\omega_z)^{1/3}$ and $F_{\delta,\nu,\eta}(x) \equiv \sum_{i,j=1}^{\infty} x^{i+j}/[i^\delta j^\nu (i+j)^\eta]$ $(x \leqslant 1)$.

The heat capacity at a given external potential and number of particles can be calculated by using

$$C = \frac{\mathrm{d}U}{\mathrm{d}T} = \left(\frac{\partial U}{\partial T}\right)_{\tilde{z}} + \left(\frac{\partial U}{\partial \tilde{z}}\right)_T \frac{\mathrm{d}\tilde{z}}{\mathrm{d}T} \tag{20}$$

where

$$\left(\frac{\partial U}{\partial T}\right)_{\tilde{z}} = k_B\left(\frac{k_B T}{\hbar\varpi}\right)^3\left\{12g_4(\tilde{z}) + \frac{a}{\lambda}[54g_{3/2}(\tilde{z})g_3(\tilde{z}) - 63F_{3/2,1/2,5/2}(\tilde{z})]\right\} \tag{21}$$

$$\left(\frac{\partial U}{\partial \tilde{z}}\right)_T = \frac{k_B T}{\tilde{z}}\left(\frac{k_B T}{\hbar\varpi}\right)^3\left\{3g_3(\tilde{z}) + \frac{a}{\lambda}[12g_{3/2}(\tilde{z})g_2(\tilde{z})\right.$$
$$\left.+12g_{1/2}(\tilde{z})g_3(\tilde{z}) - 14F_{3/2,1/2,3/2}(\tilde{z})]\right\} \tag{22}$$

and

$$\frac{\mathrm{d}z}{\mathrm{d}T} = -\frac{\tilde{z}}{T}\frac{3g_3(\tilde{z}) + \frac{a}{\lambda}[14g_{3/2}(\tilde{z})g_2(\tilde{z}) - 14F_{3/2,1/2,3/2}(\tilde{z})]}{g_2(\tilde{z}) + \frac{a}{\lambda}[4g_{3/2}(\tilde{z})g_1(\tilde{z}) + 4g_{1/2}(\tilde{z})g_2(\tilde{z}) - 4F_{3/2,1/2,1/2}(\tilde{z})]} \tag{23}$$

can be directly derived from equations (17) and (18).

It should be noted that, unlike the thermodynamic quantities [29, 30] expressed by the functions of the fugacity $z = \exp(\beta\mu) = \exp\{\beta\bar{\mu}[n(0)]\} \equiv \bar{z}[n(0)]$, the expressions of the thermodynamic quantities derived above are given by the functions of the parameter $\tilde{z} \equiv \bar{z}_0[n(0)]$, so that the divergent difficulty existing in [29, 30] is overcome. The reason is as follows: for the repulsively interacting Bose system, the fugacity z may be greater than 1, and consequently, some expressions in [29, 30] may become useless due to the divergence of $g_l(z)$ and $F_{\delta,\nu,\eta}(z)$ when the temperature approaches T_C from $T > T_C$. In contrast, because $\tilde{z} \leqslant 1$ when $T \geqslant T_C$, equations (17)–(19) and (21) are convergent in the entire region of $T \geqslant T_C$. Although $g_{1/2}(\tilde{z})$, $g_1(\tilde{z})$ and $F_{3/2,1/2,1/2}(\tilde{z})$ in equations (22) and (23) will be divergent when $\tilde{z} = 1$, it can be proved that the heat capacity given by equation (20) is still convergent.

2.2. The case of $T < T_C$

When $T < T_C$, BEC occurs in the region of $n(\boldsymbol{r}) > n_C$ or $V(\boldsymbol{r}) < V_C$, where V_C is the potential at the edge of the condensation region. In the region of $V(\boldsymbol{r}) \geqslant V_C$, all the particles are in the normal state, and consequently, the chemical potential and the densities of particles, energy and entropy can be still given by equations (4) and (9)–(11), respectively. At the edge of the condensation region, $n(\boldsymbol{r}) = n_C$, $V(\boldsymbol{r}) = V_C$ and $\bar{z}_0(n_C) = 1$, so the chemical potential can be given by

$$\mu = 4a\lambda^2 n_C k_B T + V_C. \tag{24}$$

From equations (4), (9)–(11) and (24), one can derive the densities of particles, energy and entropy outside the condensation region as

$$\begin{aligned} n_{V(\boldsymbol{r})\geqslant V_C}(\boldsymbol{r}) = \frac{1}{\lambda^3}\Big\{ & g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) + \frac{a}{\lambda}\{4\zeta(3/2)g_{1/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) \\ & - 4g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\})g_{1/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\})\}\Big\} \end{aligned} \tag{25}$$

$$\begin{aligned} u_{V(\boldsymbol{r})\geqslant V_C}(\boldsymbol{r}) = \frac{k_B T}{\lambda^3}\Big\{ & \frac{3}{2}g_{5/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) + \beta V(\boldsymbol{r})g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) \\ & + \frac{a}{\lambda}\big\{6\zeta(3/2)g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) - 4g_{3/2}^2(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) \\ & + 4\beta V(\boldsymbol{r})\zeta(3/2)g_{1/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) \\ & - 4\beta V(\boldsymbol{r})g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\})g_{1/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\})\big\}\Big\} \end{aligned} \tag{26}$$

and

$$\begin{aligned} s_{V(\boldsymbol{r})\geqslant V_C}(\boldsymbol{r}) = \frac{k_B}{\lambda^3}\Big\{ & \frac{5}{2}g_{5/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) + \beta[V(\boldsymbol{r}) - V_C]g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) \\ & + \frac{a}{\lambda}\big\{6\zeta(3/2)g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) - 6g_{3/2}^2(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) \\ & + 4\beta[V(\boldsymbol{r}) - V_C]\zeta(3/2)g_{1/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\}) - 4\beta[V(\boldsymbol{r}) \\ & - V_C]g_{3/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\})g_{1/2}(\exp\{-\beta[V(\boldsymbol{r}) - V_C]\})\big\}\Big\}. \end{aligned} \tag{27}$$

In the condensation region, $n(\boldsymbol{r}) > n_C$ and BEC occurs. The chemical potential is now given by

$$\mu = 2a\lambda^2[n(\boldsymbol{r}) + n_C]k_BT + V(\boldsymbol{r}) \tag{28}$$

according to equations (2) and (3). Thus, the density of particles

$$n_{V(\boldsymbol{r})<V_C}(\boldsymbol{r}) = n_C + \frac{\beta[V_C - V(\boldsymbol{r})]}{2a\lambda^2} \tag{29}$$

can be derived with the help of equations (24) and (28). It is seen that the density inside the condensation region consists of the contributions from the normal part with the saturated density n_C and the condensed part with the density

$$n_s(\boldsymbol{r}) = \frac{\beta[V_C - V(\boldsymbol{r})]}{2a\lambda^2}. \tag{30}$$

By using equations (5)–(8) and (29), the densities of energy and entropy inside the condensation region are found to be

$$u_{V(\boldsymbol{r})<V_C}(\boldsymbol{r}) = \frac{k_BT}{\lambda^3}\left\{\frac{3}{2}\zeta(5/2) + \frac{1}{2}\zeta(3/2)\beta[V_C + V(\boldsymbol{r})] + \frac{\lambda\beta^2\left[V_C^2 - V^2(\boldsymbol{r})\right]}{4a} + \frac{2a\zeta^2(3/2)}{\lambda}\right\} \tag{31}$$

and

$$s_{V(\boldsymbol{r})<V_C}(\boldsymbol{r}) = \frac{k_B}{\lambda^3}\left\{\frac{5}{2}\zeta(5/2) - \frac{3}{2}\zeta(3/2)\beta[V_C - V(\boldsymbol{r})]\right\}. \tag{32}$$

Finally, the total number of particles, ground-state occupation, total energy and entropy in the case of $T < T_C$ are, respectively, given by

$$\begin{aligned} N &= \int_{V(\boldsymbol{r})<V_C} n_{V(\boldsymbol{r})<V_C}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} + \int_{V(\boldsymbol{r})\geqslant V_C} n_{V(\boldsymbol{r})\geqslant V_C}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\ &= \left(\frac{k_BT}{\hbar\varpi}\right)^3\left\{h_3(\beta V_C) + \frac{2\zeta(5/2)}{\pi^{1/2}}(\beta V_C)^{1/2} + \frac{4\zeta(3/2)}{3\pi^{1/2}}(\beta V_C)^{3/2}\right. \\ &\quad \left. + \frac{4}{15\pi^{1/2}}\left(\frac{\lambda}{a}\right)(\beta V_C)^{5/2} + \frac{a}{\lambda}[4\zeta(2)\zeta(3/2) - 4F_{3/2,1/2,3/2}(1)]\right\} \end{aligned} \tag{33}$$

$$N_s = \int_{V(\boldsymbol{r})<V_C} n_s(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = \frac{4}{15\pi^{1/2}}\left(\frac{\lambda}{a}\right)\left(\frac{k_BT}{\hbar\varpi}\right)^3(\beta V_C)^{5/2} \tag{34}$$

$$\begin{aligned} U &= \int_{V(\boldsymbol{r})<V_C} u_{V(\boldsymbol{r})<V_C}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} + \int_{V(\boldsymbol{r})\geqslant V_C} u_{V(\boldsymbol{r})\geqslant V_C}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\ &= k_BT\left(\frac{k_BT}{\hbar\varpi}\right)^3\left\{3h_4(\beta V_C) + \frac{6\zeta(7/2)}{\pi^{1/2}}(\beta V_C)^{1/2} + \frac{4\zeta(5/2)}{\pi^{1/2}}(\beta V_C)^{3/2}\right. \\ &\quad + \frac{16\zeta(3/2)}{15\pi^{1/2}}(\beta V_C)^{5/2} + \frac{4}{21\pi^{1/2}}\left(\frac{\lambda}{a}\right)(\beta V_C)^{7/2} + \frac{8\zeta^2(3/2)}{3\pi^{1/2}}\left(\frac{a}{\lambda}\right)(\beta V_C)^{3/2} \\ &\quad \left. + \frac{a}{\lambda}[12\zeta(3/2)\zeta(3) - 14F_{3/2,1/2,5/2}(1)]\right\} \end{aligned} \tag{35}$$

and

$$\begin{aligned} S &= \int_{V(\boldsymbol{r})<V_C} s_{V(\boldsymbol{r})<V_C}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} + \int_{V(\boldsymbol{r})\geqslant V_C} s_{V(\boldsymbol{r})\geqslant V_C}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \\ &= k_B\left(\frac{k_BT}{\hbar\varpi}\right)^3\left\{4h_4(\beta V_C) - (\beta V_C)h_3(\beta V_C) + \frac{8\zeta(7/2)}{\pi^{1/2}}(\beta V_C)^{1/2}\right. \\ &\quad + \frac{10\zeta(5/2)}{3\pi^{1/2}}(\beta V_C)^{3/2} - \frac{4\zeta(3/2)}{5\pi^{1/2}}(\beta V_C)^{5/2} \\ &\quad \left. + \frac{a}{\lambda}[12\zeta(3/2)\zeta(3) - 18F_{3/2,1/2,5/2}(1)]\right\} \end{aligned} \tag{36}$$

where $h_l(x) \equiv \sum_{i=1}^{\infty}\exp(ix)\mathrm{erfc}[(ix)^{1/2}]/i^l$, $\mathrm{erfc}(x) = (2/\pi^{1/2})\int_x^{\infty}\exp(-t^2)\,\mathrm{d}t$ is the complementary error function. It is easy to prove that $\exp(ix)\mathrm{erfc}[(ix)^{1/2}] \leqslant 1$. Hence, $h_l(x)$ is convergent for $l > 1$, and, in particular, $h_l(0) = \zeta(l)$.

The heat capacity in the case of $T < T_C$ can be calculated by

$$C = \left(\frac{\partial U}{\partial T}\right)_{V_C} + \left(\frac{\partial U}{\partial V_C}\right)_T \frac{\mathrm{d}V_C}{\mathrm{d}T} \tag{37}$$

where

$$\begin{aligned} \left(\frac{\partial U}{\partial T}\right)_{V_C} &= k_B\left(\frac{k_BT}{\hbar\varpi}\right)^3\left\{12h_4(\beta V_C) - 3(\beta V_C)h_3(\beta V_C) + \frac{24\zeta(7/2)}{\pi^{1/2}}(\beta V_C)^{1/2}\right. \\ &\quad + \frac{10\zeta(5/2)}{\pi^{1/2}}(\beta V_C)^{3/2} + \frac{8\zeta(3/2)}{5\pi^{1/2}}(\beta V_C)^{5/2} + \frac{8\zeta^2(3/2)}{\pi^{1/2}}\left(\frac{a}{\lambda}\right)(\beta V_C)^{3/2} \\ &\quad \left. + \frac{a}{\lambda}[54\zeta(3/2)\zeta(3) - 63F_{3/2,1/2,5/2}(1)]\right\} \end{aligned} \tag{38}$$

$$\begin{aligned} \left(\frac{\partial U}{\partial V_C}\right)_T &= \left(\frac{k_BT}{\hbar\varpi}\right)^3\left\{3h_3(\beta V_C) + \frac{6\zeta(5/2)}{\pi^{1/2}}(\beta V_C)^{1/2} + \frac{8\zeta(3/2)}{3\pi^{1/2}}(\beta V_C)^{3/2}\right. \\ &\quad \left. + \frac{2}{3\pi^{1/2}}\left(\frac{\lambda}{a}\right)(\beta V_C)^{5/2} + \frac{4\zeta^2(3/2)}{\pi^{1/2}}\left(\frac{a}{\lambda}\right)(\beta V_C)^{1/2}\right\} \end{aligned} \tag{39}$$

and

$$\begin{aligned} \frac{\mathrm{d}V_C}{\mathrm{d}T} &= -\frac{V_C}{T}\left\{3h_3(\beta V_C) - \left(\frac{V_C}{kT}\right)h_2(\beta V_C) + \frac{6\zeta(5/2)}{\pi^{1/2}}(\beta V_C)^{1/2}\right. \\ &\quad \left. + \frac{2\zeta(3/2)}{\pi^{1/2}}(\beta V_C)^{3/2} + \frac{a}{\lambda}[14\zeta(2)\zeta(3/2)] - 14F_{3/2,1/2,3/2}(1)\right\} \\ &\quad \left\{(\beta V_C)h_2(\beta V_C) + \frac{2\zeta(3/2)}{\pi^{1/2}}(\beta V_C)^{3/2} + \frac{2}{3\pi^{1/2}}\left(\frac{\lambda}{a}\right)(\beta V_C)^{5/2}\right\}^{-1} \end{aligned} \tag{40}$$

can be derived from equations (33) and (35).

It should be noted that the present paper mainly concentrates on the effects of interactions on the behaviour of an imperfect Bose gas and does not consider the effects of finite number of particles, that is, all the above results are derived under the thermodynamic limit. It has been shown that the corrections to the thermodynamic quantities due to finite particles are of the order of $1/N^{1/3}$ at $T < T_C$ [31, 32], which can be neglected for a system of large number of particles.

3. Discussion

(1) From equations (13) and (18)–(20), it can be clearly seen that, when $T \geqslant T_C$, the lowest order corrections to the thermodynamic quantities due to the interactions are of the order of a/λ, which is small for the weak interactions. When $a = 0$ is set, equations (13) and (18)–(20), respectively, become the expressions of chemical potential, total energy, entropy and heat capacity of the corresponding non-interacting system at $T \geqslant T_C$ [33].

(2) It can be derived from equation (34) that

$$V_C = \eta k_B T_{C0} f_s^{5/2} \tag{41}$$

where $T_{C0} = (\hbar\varpi/k_B)[N/\zeta(3)]^{1/3}$ is the critical temperature of BEC for the corresponding non-interacting Bose system, $f_s = N_s/N$ is the ground-state fraction, which can be determined according to equations (33) and (34),

$$\eta = \frac{15^{2/5}\zeta^{1/3}(3)}{2} N^{1/15}\left(\frac{a}{a_h}\right)^{2/5} \approx 1.57 N^{1/15}\left(\frac{a}{a_h}\right)^{2/5} \tag{42}$$

is a parameter related to the strength of interactions [23, 24] and $a_h = \sqrt{\hbar/m\varpi}$ is the characteristic length of the harmonic potential. Substituting equation (41) into equations (24) and (35)–(40) and expanding these equations with respect to η, we can derive the chemical potential, total energy, entropy and heat capacity at $T < T_C$ as

$$\mu = k_B T_{C0}\left[f_s^{2/5}\eta + \frac{16\zeta(3/2)}{15\pi^{1/2}\zeta(3)} t^{3/2}\eta^{5/2}\right] \tag{43}$$

$$\begin{aligned} U = Nk_B T_{C0}\Bigg\{ & \frac{3\zeta(4)}{\zeta(3)}t^4 + \left(3t^3 + \frac{5}{7}f_s\right) f_s^{2/5}\eta + \frac{3\zeta(2)}{2\zeta(3)} t^2 f_s^{4/5}\eta^2 \\ & + \frac{8\zeta(2/3)}{15\pi^{1/2}\zeta(3)} t^{3/2}\left\{\left[6 - \frac{7F_{3/2,1/2,5/2}(1)}{\zeta(3/2)\zeta(3)}\right]t^3 - f_s\right\}\eta^{5/2}\Bigg\} \end{aligned} \tag{44}$$

$$\begin{aligned} S = Nk_B\Bigg\{ & \frac{4\zeta(4)}{\zeta(3)}t^3 + 3t^2 f_s^{2/5}\eta + \frac{\zeta(2)}{\zeta(3)} t f_s^{4/5}\eta^2 \\ & + \frac{8\zeta(2/3)}{5\pi^{1/2}\zeta(3)} t^{1/2}\left\{\left[2 - \frac{3F_{3/2,1/2,5/2}(1)}{\zeta(3/2)\zeta(3)}\right]t^3 - f_s\right\}\eta^{5/2}\Bigg\} \end{aligned} \tag{45}$$

and

$$\begin{aligned} C = Nk_B\Bigg\{ & \frac{12\zeta(4)}{\zeta(3)}t^3 + 6t^2 f_s^{2/5}\left(1 - \frac{3}{5}\frac{t^3}{f_s}\right)\eta + \frac{\zeta(2)}{\zeta(3)} t f_s^{4/5}\left(1 - \frac{24}{5}\frac{t^3}{f_s} + \frac{36}{25}\frac{t^6}{f_s^2}\right)\eta^2 \\ & + \frac{4\zeta(2/3)}{5\pi^{1/2}\zeta(3)} t^{1/2}\left\{\left[20 - \frac{21F_{3/2,1/2,5/2}(1)}{\zeta(3/2)\zeta(3)}\right]t^3 - f_s\right\}\eta^{5/2}\Bigg\}. \end{aligned} \tag{46}$$

It is seen that equations (43) and (44) are just the same as the corresponding results in [23, 24] if f_s is replaced approximately by $1 - t^3$ and only the lowest order corrections from the interactions are considered.

It is seen from equations (43)–(46) that the lowest order corrections from the interactions are of the order of $\eta \sim (a/a_h)^{2/5}$ at $T < T_C$. They are much larger than the corresponding corrections at $T \geqslant T_C$, which are linear in $a/\lambda \sim a/a_h$. The result can be physically explained as follows: at low temperatures, the particles are

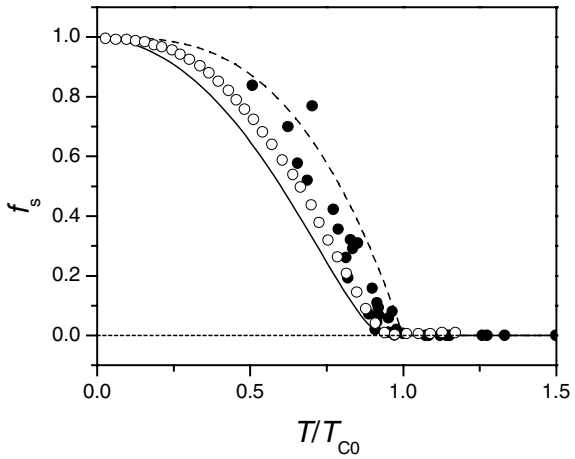

Figure 1. The ground-state fraction as a function of temperature. Solid, long-dashed and short-dashed lines represent our results for an interacting Bose gas, non-interacting Bose gas and Maxwell–Boltzmann gas, respectively. The solid circles are the experimental data of Ensher *et al* [9]. The empty circles are the numerical results of Minguzzi *et al* [20].

more densely concentrated around the centre of the potential, so the effects due to the interatomic forces, which is proportional to the density of particles, will become stronger. When $a = 0$, i.e., $\eta = 0$, the above equations, respectively, become the expressions of the chemical potential, total energy, entropy and heat capacity of the corresponding non-interacting system at $T < T_C$ [33].

(3) According to equations (13), (17)–(24) and (33)–(40), one can expound the dependences of f_s, μ, U, S and C on the temperature in detail, as shown in figures 1–5, respectively, where the parameters given experimentally by Ensher *et al* [9] are taken, i.e., $\omega_z = 2343.63$ (s^{-1}), $\omega_x = \omega_y = \omega_z/\sqrt{8}$, $m = 87$ (au), $N = 40\,000$, $a = 110a_B$ and a_B is the Bohr radius.

Figure 1 shows the curves of the ground-state fraction f_s varying with the scaled temperature T/T_{C0}. It is seen that both the ground-state fraction and the critical temperature decrease significantly with respect to the values predicted by the non-interacting theory. The result is as expected, since the repulsive forces between the particles may weaken the effect of the external potential in concentrating the particles around the centre and make BEC more difficult. By setting $\tilde{z} = 1$ in equation (17) or $V_C = 0$ in equation (33), one can find the critical temperature

$$T_C \approx T_{C0}\left\{1 - \frac{4a}{3\lambda_{C0}}\left[\frac{\zeta(2)\zeta(3/2)}{\zeta(3)} - \frac{F_{3/2,1/2,3/2}(1)}{\zeta(3)}\right]\right\} \tag{47}$$

where $\lambda_{C0} = \sqrt{2\pi\hbar^2/mk_BT_{C0}}$. Equation (47) coincides with the result in [21]. For the parameters given above, $T_C \approx 0.94T_{C0}$. The value is in good agreement with the experimental data [9] and numerical results [20–22].

Figure 2 presents the dependence of the chemical potential on temperature, which is found to agree well with the numerical result obtained by Giorgini *et al* [21, 22]. It is seen that, unlike the non-interacting Bose system, for which $\mu = 0$ when $T \leqslant T_{C0}$, the chemical potential of the repulsively interacting system below the critical temperature is greater than

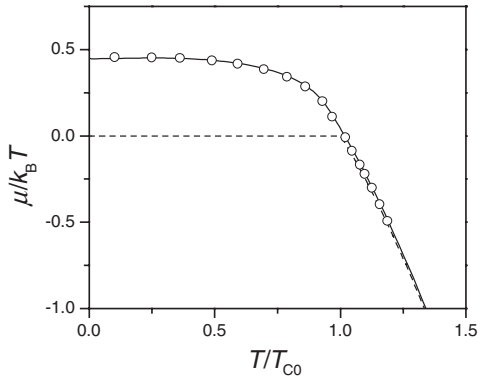

Figure 2. The chemical potential as a function of temperature. Solid and dashed lines represent our results for an interacting Bose gas and non-interacting Bose gas, respectively. The empty circles are the numerical results of Giorgini *et al* [22].

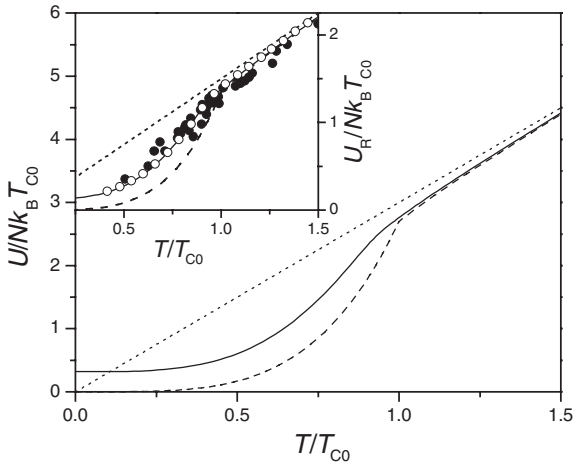

Figure 3. The total energy and release energy (inset) as a function of temperature. Solid, long-dashed and short-dashed lines represent our results for an interacting Bose gas, non-interacting Bose gas and Maxwell–Boltzmann gas, respectively. The solid circles are the experimental data of Ensher *et al* [9]. The empty circles are the numerical results of Minguzzi *et al* [20].

zero. One can estimate from equation (43) that when $T \to 0$,

$$\mu = \eta k T_{C0} = \frac{\hbar\varpi}{2}\left(\frac{15Na}{a_h}\right)^{2/5}. \tag{48}$$

The result is consistent with that of the Ginzburg–Pitaevskii–Gross mean field theory [34].

Figure 3 gives the total energy as a function of temperature. It is indicated that the interatomic forces substantially increase the total energy of the system below the critical temperature. The ground-state energy can be obtained from equation (44) as

$$U = \frac{5}{7}\eta k T_{C0} = \frac{5\hbar\varpi}{14}\left(\frac{15Na}{a_h}\right)^{2/5}. \tag{49}$$

It is in accordance with the result in [34]. The inset of figure 3 gives the curve of the release energy U_R (defined as the energy of the system after the external potential has been switched

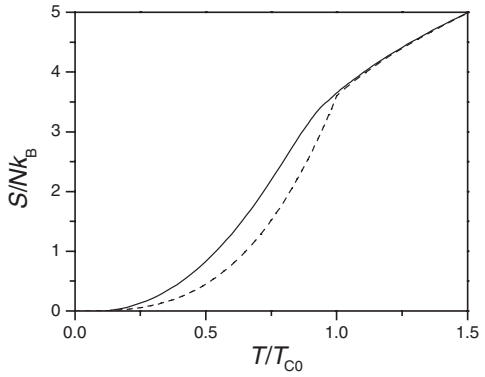

Figure 4. The entropy as a function of temperature. Solid and dashed lines represent our results for an interacting Bose gas and non-interacting Bose gas, respectively.

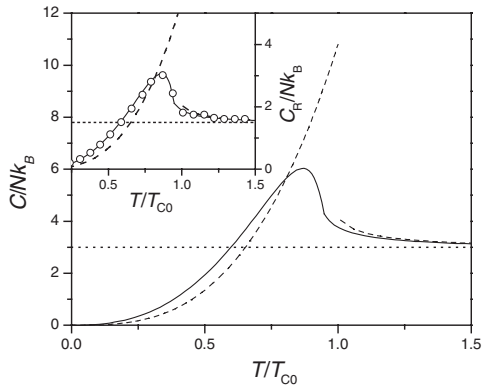

Figure 5. The heat capacity and release heat capacity (inset) as a function of temperature. Solid, long-dashed and short-dashed lines represent our results for an interacting Bose gas, non-interacting Bose gas and Maxwell–Boltzmann gas, respectively. The empty circles are the numerical results of Minguzzi *et al* [20].

off [20]) versus temperature, which is compared with the experimental data obtained by Ensher *et al* [9] and the result of the two-fluid mean-field model established by Minguzzi *et al* [20]. It is seen that the result agrees well with the experimental data and almost reproduces the numerical result obtained by Minguzzi *et al*.

Figure 4 shows the curve of the entropy varying with temperature, which is compared with the prediction of non-interacting theory. As expected, the effects of interactions on the entropy are significant when $T < T_C$, but very small when $T \geqslant T_C$.

Finally, the curves of the heat capacities versus temperature are plotted in figure 5. It is interesting to note that in the region of $T < T_C$, the heat capacity does not increase monotonically with T, like that of the non-interacting system. After reaching the maximum at a certain temperature T_m near T_C, the value of C decreases quickly when T approaches T_C from T_m. The inset of figure 5 shows the curve of the release heat capacity C_R (defined as $C_R = \partial U_R/\partial T$) versus temperature, which is compared with the result obtained by Minguzzi *et al* [20]. Good agreement can be clearly seen.

4. Conclusions

We have obtained an analytical description for the low temperature behaviour of a trapped interacting Bose gas by using the principle of the constancy of chemical potentials in equilibrium and the local-density approximation. The expressions of several thermodynamic quantities are derived, in which the corrections due to the interactions between the particles are given explicitly. The divergent problem existing in some papers is overcome. It is more important that the analytical results derived by a conceptually simple method are in good agreement with the experimental data and the numerical predictions, and many significant conclusions in the literature are included in the present paper.

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